

# PATENT COOPERATION TREATY

# PCT

## INTERNATIONAL SEARCH REPORT

(PCT Article 18 and Rules 43 and 44)

Applicant's or agent's file reference  WP-1859-P1	<b>FOR FURTHER ACTION</b> see Notification of Transmittal of International Search Report (Form PCT/ISA/220) as well as, where applicable, item 5 below.	
International application No.  PCT/CH 03/00548	International filing date (day/month/year)  14/08/2003	(Earliest) Priority Date (day/month/year)  27/08/2002
Applicant  BARTELS, Christian		

This International Search Report has been prepared by this International Searching Authority and is transmitted to the applicant according to Article 18. A copy is being transmitted to the International Bureau.

This International Search Report consists of a total of 4 sheets.

☒ It is also accompanied by a copy of each prior art document cited in this report.

**1. Basis of the report**

a. With regard to the **language**, the international search was carried out on the basis of the international application in the language in which it was filed, unless otherwise indicated under this item.

☐ the international search was carried out on the basis of a translation of the international application furnished to this Authority (Rule 23.1(b)).

b. With regard to any **nucleotide and/or amino acid sequence** disclosed in the international application, the international search was carried out on the basis of the sequence listing:

☐ contained in the international application in written form.

☐ filed together with the international application in computer readable form.

☐ furnished subsequently to this Authority in written form.

☐ furnished subsequently to this Authority in computer readable form.

☐ the statement that the subsequently furnished written sequence listing does not go beyond the disclosure in the international application as filed has been furnished.

☐ the statement that the information recorded in computer readable form is identical to the written sequence listing has been furnished

2. ☐ **Certain claims were found unsearchable** (See Box I).

3. ☐ **Unity of invention is lacking** (see Box II).

4. With regard to the **title**,

☒ the text is approved as submitted by the applicant.

☐ the text has been established by this Authority to read as follows:

5. With regard to the **abstract**,

☒ the text is approved as submitted by the applicant.

☐ the text has been established, according to Rule 38.2(b), by this Authority as it appears in Box III. The applicant may, within one month from the date of mailing of this international search report, submit comments to this Authority.

6. The figure of the **drawings** to be published with the abstract is Figure No.

☒ as suggested by the applicant.

☐ because the applicant failed to suggest a figure.

☐ because this figure better characterizes the invention.

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☐ None of the figures.

## INTERNATIONAL SEARCH REPORT

International Application No

PCT/CH 03/00548

**A. CLASSIFICATION OF SUBJECT MATTER**  
 IPC 7 G06F17/18

According to International Patent Classification (IPC) or to both national classification and IPC

**B. FIELDS SEARCHED**

Minimum documentation searched (classification system followed by classification symbols)

IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal

**C. DOCUMENTS CONSIDERED TO BE RELEVANT**

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>BARTELS C ET AL: "MULTIDIMENSIONAL ADAPTIVE UMBRELLA SAMPLING: APPLICATIONS TO MAIN CHAIN AND SIDE CHAIN PEPTIDE CONFORMATIONS"</p> <p>JOURNAL OF COMPUTATIONAL CHEMISTRY, JOHN WILEY AND SONS, CHICHESTER, GB, vol. 18, no. 12, 1997, pages 1450-1462, XP001124375</p> <p>ISSN: 0192-8651</p> <p>the whole document</p> <p style="text-align: center;">----- -/--</p>	1-12

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

## \* Special categories of cited documents:

- \*A\* document defining the general state of the art which is not considered to be of particular relevance
- \*E\* earlier document but published on or after the international filing date
- \*L\* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- \*O\* document referring to an oral disclosure, use, exhibition or other means
- \*P\* document published prior to the international filing date but later than the priority date claimed

\*T\* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention

\*X\* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

\*Y\* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.

\*G\* document member of the same patent family

Date of the actual completion of the international search

14 October 2004

Date of mailing of the international search report

21/10/2004

Name and mailing address of the ISA

European Patent Office, P.B. 5818 Patentlaan 2  
 NL - 2280 HV Rijswijk  
 Tel. (+31-70) 340-2040, Tx. 31 651 epo nl,  
 Fax: (+31-70) 340-3016

Authorized officer

Domingo Vecchioni, M

## INTERNATIONAL SEARCH REPORT

International Application No

PCT/CH 03/00548

## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
A	<p>BARTELS C ET AL: "DETERMINATION OF EQUILIBRIUM PROPERTIES OF BIOMOLECULAR SYSTEMS USING MULTIDIMENSIONAL ADAPTIVE UMBRELLA SAMPLING" JOURNAL OF CHEMICAL PHYSICS, NEW YORK, NY, US, vol. 111, no. 17, 1 November 1999 (1999-11-01), pages 8048-8067, XP008012543 ISSN: 0021-9606 the whole document</p>	1-12
A	<p>HEINZ T N ET AL: "COMPARISON OF FOUR METHODS TO COMPUTE THE DIELECTRIC PERMITTIVITY OF LIQUIDS FROM MOLECULAR DYNAMICS SIMULATIONS" JOURNAL OF CHEMICAL PHYSICS, NEW YORK, NY, US, vol. 115, no. 3, 15 July 2001 (2001-07-15), pages 1125-1136, XP008012039 ISSN: 0021-9606 page 1126, right-hand column, last paragraph - page 1129, left-hand column, last paragraph</p>	1-12
A	<p>US 5 148 365 A (DEMBO RON S) 15 September 1992 (1992-09-15)</p>	

## INTERNATIONAL SEARCH REPORT

### Information on patent family members

International Application No

PCT/CH 03/00548

Patent document cited in search report	Publication date	Patent family member(s)	Publication date
US 5148365	A	15-09-1992	NONE